

JS 9/15/21
RJA 01/18/22

Fate Report for Case # P-18-0152

Fate

Summary Statement

Fate P-18-0152

Summary FATE:

Statement: Estimations for the low weight, monomer species, MW = [REDACTED]

[REDACTED] with MP < 25 °C (E)

log Kow = -1.41 (E)

S

> 10 g/L at 25 °C (E)

VP = 1.2E-4 torr at 25 °C (E)

BP = 292 °C

(E)

H < 1.00E-8 (E)

log Koc = 2.60 (E)

log Fish BCF = 0.50 (3)

(E)

log Fish BAF = -0.05 (1) (E)

POTW removal (%) = 0-25 via

sorption; Analog [REDACTED] OECD 301B(Mod Sturm CO2 ev):

3.22-6.89%/29 d. NRB.

Time for complete ultimate aerobic biodeg > mo

Sorption to soils/sediments = moderate

PBT Potential:

P3B1

*CEB FATE: Migration to ground water = moderate

Bioconcentration factor to be put into E-FAST: 1

PMN

Material:

Overall wastewater treatment removal is 0-25% via sorption.

Sorption to sludge is low based on estimated physical-chemical properties from EPISUITE.

Air Stripping (Volatilization to air) is

negligible based on estimated physical-chemical properties from EPISUITE.

Removal by biodegradation in wastewater treatment is negligible based on the measured data for an analog [REDACTED]: OECD 301B(Mod Sturm CO2 ev): 3.22-6.89%/29d NRB).

The aerobic aquatic biodegradation

half-life is greater than months based on the measured data for an analog

[REDACTED] OECD 301B(Mod Sturm CO2 ev): 3.22-6.89%/29d NRB).

The

anaerobic aquatic biodegradation half-life is greater than months based on

the aerobic biodegradation half-life. The anaerobic biodegradation half-life is projected to be greater than or equal to the aerobic biodegradation half-life.

Sorption to soil and sediment is moderate based on estimated physical-chemical properties from EPISUITE.

Migration to groundwater is moderate based on estimated physical-chemical properties from EPISUITE.

PMN Material:

High

Persistence (P3) is based on the aerobic and anaerobic biodegradation half-lives.

Low Bioaccumulation potential (B1) is based on BCFBAF model estimates.

Bioconcentration/Bioaccumulation factor to be put into E-Fast: 1.

CBI: [REDACTED]

Fate Lee, WenHsiung

Assessor:

SMILES: [REDACTED]

Physical Properties

Property	Measured/Calculated Value	EPI
Molecular Form:	[REDACTED]	[REDACTED]
Molecular Wt.:	[REDACTED]	[REDACTED]
% < 500:	[REDACTED]	
% < 1000:	[REDACTED]	

Property	Measured Value	Method	Estimated Value	Method	EPI
Melting Point:					NaN °C (Exp.) 282.0794982910156 °C (Est., Joback) 119.01715087890625 °C (Est., Gold) 151.62960815429688 °C (Est., Selected)
Boiling Point:			327		1.9112759042637781% NaN °C (Exp.) 398.49 °C (Est.)

Property	Measured Value	Method	Estimated Value	Method	EPI
BP Pressure: Vapor Pressure:			0.000012		671.6512451171875 °K (Est.)
					NaN mmHg (Exp.)
					8.776204236904395E-8 Pa (Est., Antoine)
					6.582712708258498E-10 mmHg (Est., Antoine)
					5.925547576351211E-7 Pa (Est., Grain)
					4.444538468033191E-9 mmHg (Est., Grain)
					1.3811481717325024E-4 Pa (Est., Mackay)
					1.0359491844800576E-6 mmHg (Est., Mackay)
					5.925547576351211E-7 Pa (Est., Selected)
					4.444538468033191E-9 mmHg (Est., Selected)
Water Solubility:			1000		1.155788608437547E-5 Pa (Est., SubCooled)
					8.669151441154099E-8 mmHg (Est., SubCooled)
					NaN (Exp.)
					3518.090087890625 (Est.)
Log P: Log Kow: Log Koc:	NaN		-1.41		NaN (Exp.)
					1.21 (Est.)
					12.086405502072507 (Est., log (MCI))
					2.7278528408647205 (Est., log (Kow))
					177443.140625 L/kg (Est., MCI)
					15.300000190734863 L/kg (Est., Kow)

Property	Measured Value	Method	Estimated Value	Method	EPI
Log BCF:					3.16 L/kg wet-wt
Henry's Law:					NaN atm-m ³ /mole (Exp.)
					2.6262408007069256E-19 atm-m ³ /mole (Est., Bond)
					0.0 atm-m ³ /mole (Est., Group)
pH:					
pH					
Comment:					

Fate Analysis

Hydrolysis (t1/2, da):		Volatilization (t1/2)		Volatilization (t1/2)	
Atm Ox	0.05200538106753519	- River (hr):		- Lake (da):	
Potential		Atm Ox	0.0	Atm Ox	
(t1/2)OH		Potential		Potential	
(hr):		(t1/2)O3		(t1/2) Total	
MITI	0.30000001192092896	(hr):		(hr):	
Linear:		MITI	0.0		
Biodeg	1.100000023841858	NonLinear:			
Linear:		Biodeg	0.8999999761581421		
Biodeg	2.5999999046325684	NonLinear:			
Survey		Biodeg	3.5		
ult:		Survey Prim:			
STP (%)	1.9112759042637781%	STP (%)	0.092710892425102%		
removal)		removal)			
Total:		Biodeg:			
STP (%)	1.818569329539617%	STP (%)	1.4935728189854662E-		
removal)		removal) 14%			
Ads:		Air:			

Rationales

Removal in Wastewater Treatment:
Atmospheric Oxidation:
Hydrolysis:
Photolysis:
Aerobic Biodegradation:

Anaerobic Biodegradation: Sorption to Soil and Sediment: Migration to Groundwater: Persistence - Air: Persistence - Water: Volatilization from Water: Soil: Sediment: Other: Standard: Bioaccumulation:
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PBT Ratings

Persistence	Bioaccumulation	Toxicity	PBT Comments
3	1		

Exposure-Based Testing

Exposure-Based Testing:

Fate Ratings

Removal in WWT/POTW

(Overall):

Removal in 0-25 WWT/POTW (Overall):

Condition	Rating Values	Rating Description				Comment
		1	2	3	4	
WWT/POTW Sorption:	1	Low	Moderate	Strong	V. Strong	
WWT/POTW Stripping:	4	Extensive	Moderate	Low	Negligible	
Biodegradation Removal:	4	Unknown	High	Moderate	Negligible	
Biodegradation Destruction:		Unknown	Complete	Partial	—	
	4		Weeks	Months		

Condition	Rating Values	Rating Description				Comment
		1	2	3	4	
Aerobic Biodeg Ult:		<= Days			> Months	
Aerobic Biodeg Prim:		<= Days	Weeks	Months	> Months	
Anaerobic Biodeg Ult:	4	<= Days	Weeks	Months	> Months	
Anaerobic Biodeg Prim:		<= Days	Weeks	Months	> Months	
Hydrolysis (t1/2 at pH 7,25C) A:		<= Minutes	Hours	Days	>= Months	
Hydrolysis (t1/2 at pH 7,25C) B:		<= Minutes	Hours	Days	>= Months	
Sorption to Soils/Sediments:	3	V. Strong	Strong	Moderate	Low	
Migration to Ground Water:	3	Negligible	Slow	Moderate	Rapid	
Photolysis A, Direct:		Negligible	Slow	Moderate	Rapid	
Photolysis B, Indirect:		Negligible	Slow	Moderate	Rapid	
Atmospheric Ox A, OH:		Negligible	Slow	Moderate	Rapid	
Atmospheric Ox B, O3:		Negligible	Slow	Moderate	Rapid	

Bio**Comments:**

Bio The EPI output file for
Comments: the PMN material with manually entered properties is attached.

Composition by [REDACTED]

[REDACTED] The submitter also stated that the product distribution depended on the [REDACTED]

A fate study summary is available. Fish log BAF = -0.05 (1).

Fate Comments:

Fate Comments: Analog [REDACTED]: OECD 301B(Mod Sturm CO2 ev): 3.22-6.89%/29 d. NRB.

**Comments/Telephone
Log**

Artifact	Update/Upload Time
	